Theory of Scattering of Molecules by Surfaces

Joseph R. Manson, Clemson University, DMR Award # 0089503

One way to study the fundamental properties of surfaces and to gain understanding of chemical reactions on surfaces is to examine the scattering of well-defined beams of molecules.

In this work we developed the theory which can be used as a mathematical framework for explaining such molecular beam experiments. The theory treats the translational and rotational motion with classical mechanics, while the excitation of internal molecular vibrational modes is treated with quantum mechanics. [Initial results published by Iftimia and Manson, Physical Review Letters **87**, 093201 (2001).]

Figure 1 shows, in a polar plot for a beam incident at a 60^0 angle, our calculations for the intensity as a function of final scattering angle (colored points) compared with experimental measurements (black lines) for the case of acetylene scattering from a clean lithium fluoride surface at three different incident energies. Figure 2 gives a comparison with experiment (blue points) for the final rotational temperature of scattered acetylene molecules as a function of incident energy. The agreement between theory and experiment indicates that we have a good understanding of the basic mechanisms for energy transfer between the molecular gas and the surface. [Experimental data by Francisco et al., Physical Review Letters **77**, 1402 (1996).]

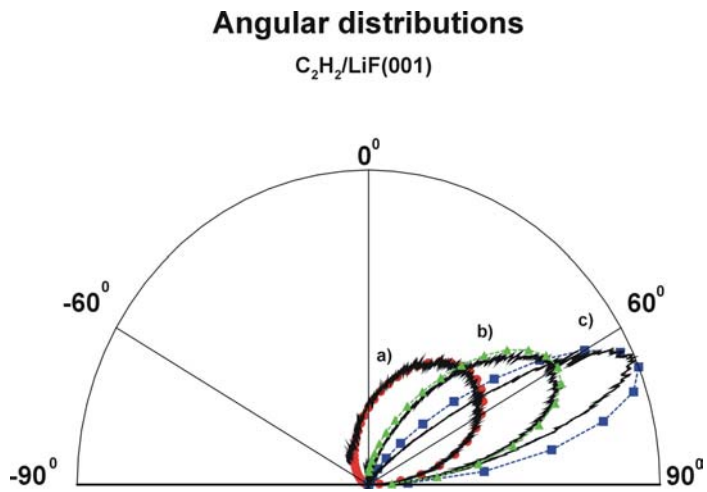

Figure 1. E_i=110meV (a); 275 (b); 618 (c).

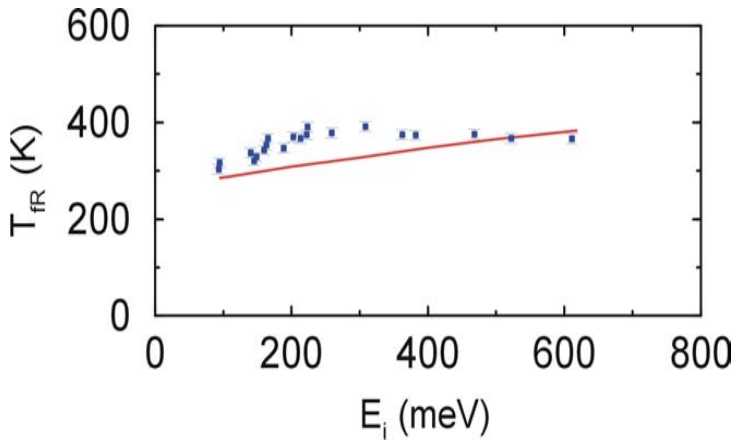

Figure 2. Rotational temperature vs. E_i.

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Educational activities:

Postdoc:

The theoretical calculations described in the page above were primarily carried out by postdoctoral research associate, Ileana Iftimia.

Graduate students:

Three graduate students also worked on this project, Jinze Dai, Yarong Tang and Mubing Li.

Undergraduate students:

A closely related project on theoretical calculations of charged ion scattering from surfaces has been carried out by undergraduate student, Judson Powers, whose work is currently supported in part by a REU supplement to this NSF grant.

Figure 3. From left to right: Ileana Iftimia, postdoc, Jinze Dai, grad student; Kirk Freeman, undergraduate, Yarong Tang, graduate student; Mubing Li, grad student; Dick Manson; Judson Powers, undergraduate; and Kenneth Pestka, grad student.